

# **Fast Computation of the Riemann Zeta Function to Arbitrary Accuracy**

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# The Players

$$s = \sigma + it$$

$$\zeta(s) = \sum_{n=1}^{\infty} n^{-s}, \quad \sigma > 1$$

$$\begin{aligned} \chi(s) &= \frac{\zeta(s)}{\zeta(1-s)} \\ &= \pi^{s-1/2} \frac{\Gamma((1-s)/2)}{\Gamma(s/2)} \end{aligned}$$

Note  $\chi(s)$  has poles at  $s = 1, 3, \dots, 2n+1, \dots$

$$Z(t) = \frac{\zeta(1/2 + it)}{\sqrt{\chi(1/2 + it)}}$$

If  $t \in \mathbb{R}$  then  $|Z(t)| = |\zeta(1/2 + it)|$  and  $Z(t) \in \mathbb{R}$ .

# Motivation

The Lagarias-Odlyzko “analytic algorithm” for  $\pi(x)$  [LO87, Gal99] requires many precise values of  $\zeta(\sigma + it)$ , with  $\sigma$  fixed,  $\sigma > 1$ . E.g. to compute  $\pi(10^{24})$  it would suffice to compute  $\zeta(1.2 + ikh)$  to roughly 45 digit precision, with

$$h = 0.0075$$

$$0 \leq k \leq 1.6 \times 10^{15}$$

$$\text{(i.e. } 0 \leq t \leq 1.2 \times 10^{13}\text{)}$$

# Euler-Maclaurin Summation

$$\begin{aligned}\zeta(s) &= \sum_{n=1}^N n^{-s} + \frac{N^{1-s}}{s-1} \\ &\quad + \sum_{m=1}^{M-1} \frac{B_m}{m} \binom{s+m-2}{m-1} N^{1-m-s} \\ &\quad + O_M(s^M N^{1-M-s})\end{aligned}$$

## Advantages

- Error analysis is straightforward [CO92].
- Allows arbitrary accuracy.
- $O(t^{1+\epsilon} + d^{1+\epsilon})$  operations to find  $d$  digits.

## Disadvantages

- $N \gtrsim t$ .
- Needs Bernoulli numbers.

# Riemann-Siegel Formula

$$Z(t) = 2 \sum_{n=1}^N n^{-1/2-it} / \sqrt{\chi(1/2 + it)} \\ + \sum_{m=0}^{M-1} \dots + O(t^{-1/4-M/2}) \quad \text{as } t \rightarrow \infty,$$

where  $N = \lfloor \sqrt{t/(2\pi)} \rfloor$ .

## Advantages

- $N \approx \sqrt{t/(2\pi)}$  for large  $t$ .

## Disadvantages

- Error analysis is difficult (currently only available for  $\sigma = 1/2$ ) [Gab79].
- Accuracy is limited.

# Quadrature Near Saddle Point

Use numerical quadrature instead of the asymptotic expansion developed in the Riemann-Siegel formula:

## Advantages

- $N \approx \sqrt{t/(2\pi)}$  for large  $t$ .
- Error analysis is straightforward.
- Allows arbitrary accuracy.

## Disadvantages

- $O(t^{1/2+\epsilon} + d^{3/2+\epsilon})$  operations to find  $d$  digits. [The Euler-Maclaurin formula wins when *very* high accuracy is needed.]

## An Integral for $\zeta(s)$

Let

$$I_N(s) = \int_{N \nearrow N+1} \frac{\exp(i\pi z^2) z^{-s}}{e^{i\pi z} - e^{-i\pi z}} dz,$$

then

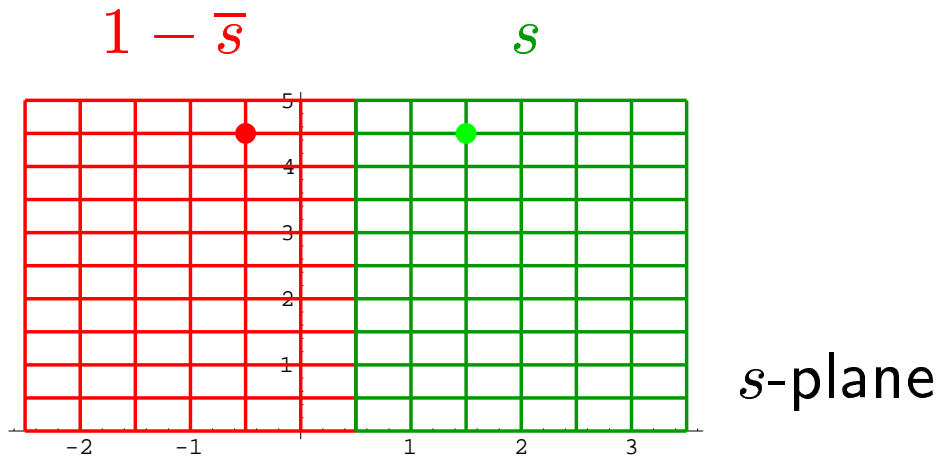
$$\zeta(s) = I_0(s) + \chi(s) \overline{I_0(1 - \bar{s})}.$$

We then use

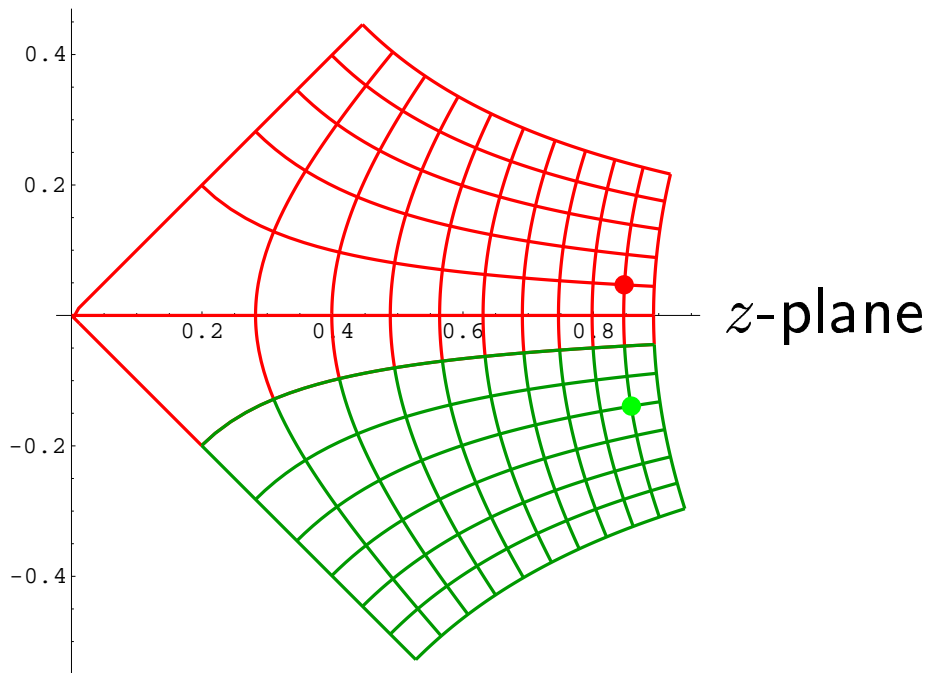
$$I_0(s) = \sum_{n=1}^N n^{-s} + I_N(s)$$

and choose  $N$  so the path is near the saddle point of  $\exp(i\pi z^2)z^{-s}$  at  $z = \sqrt{s/(2\pi i)}$ .

# Location of saddle point(s)

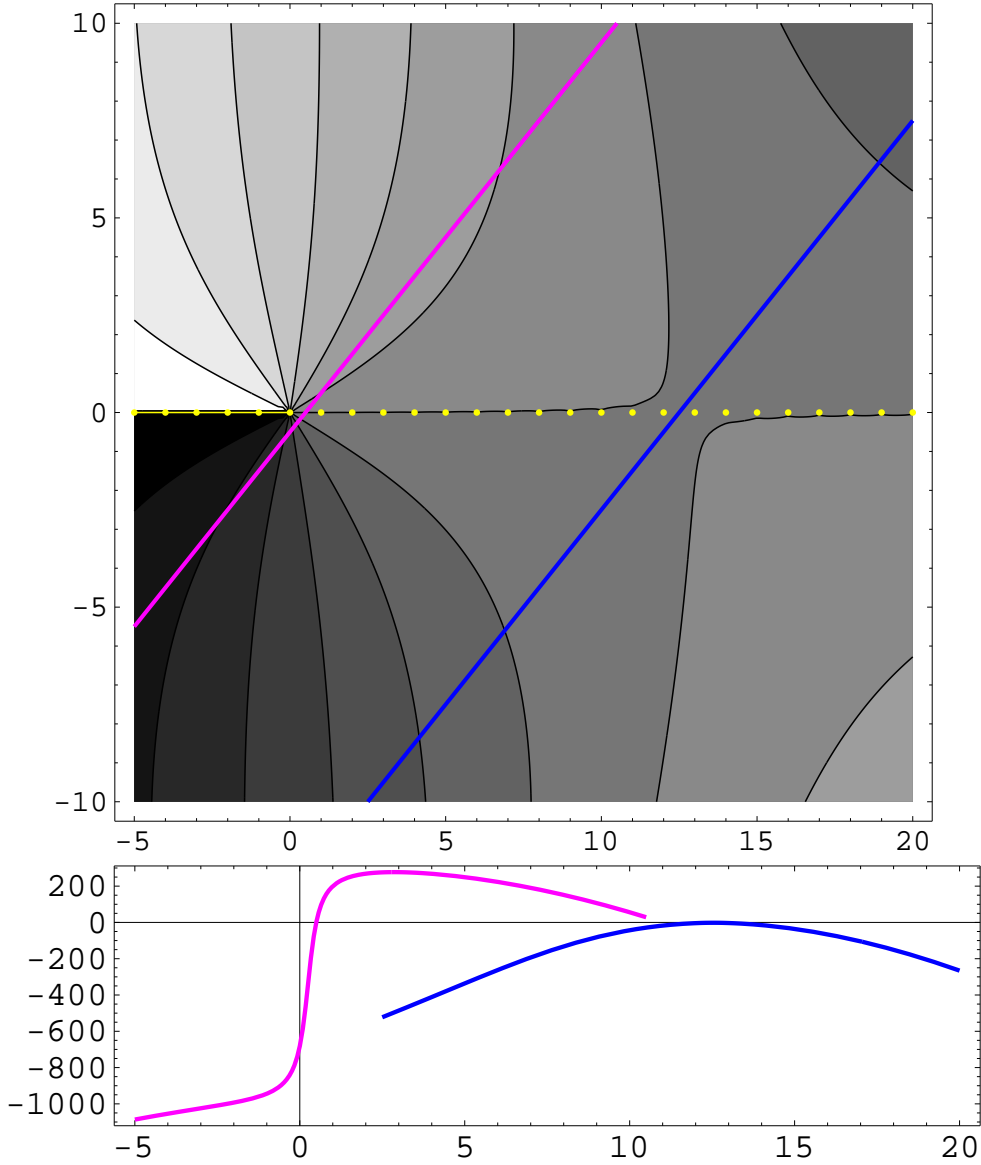


$$z = \sqrt{s/(2\pi i)}$$





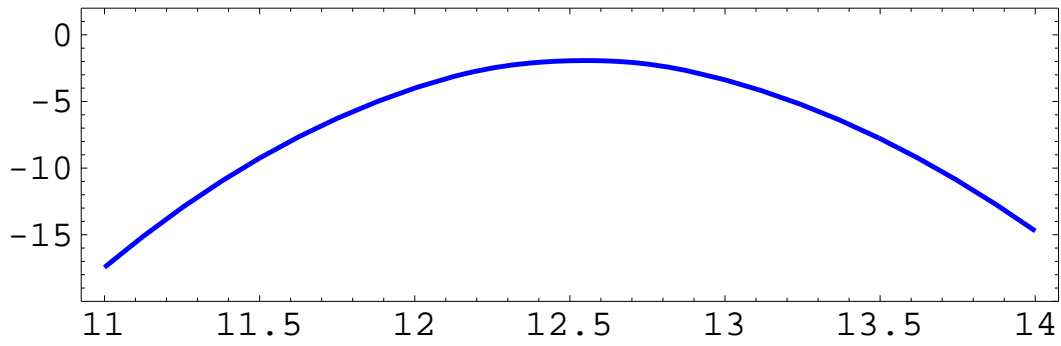
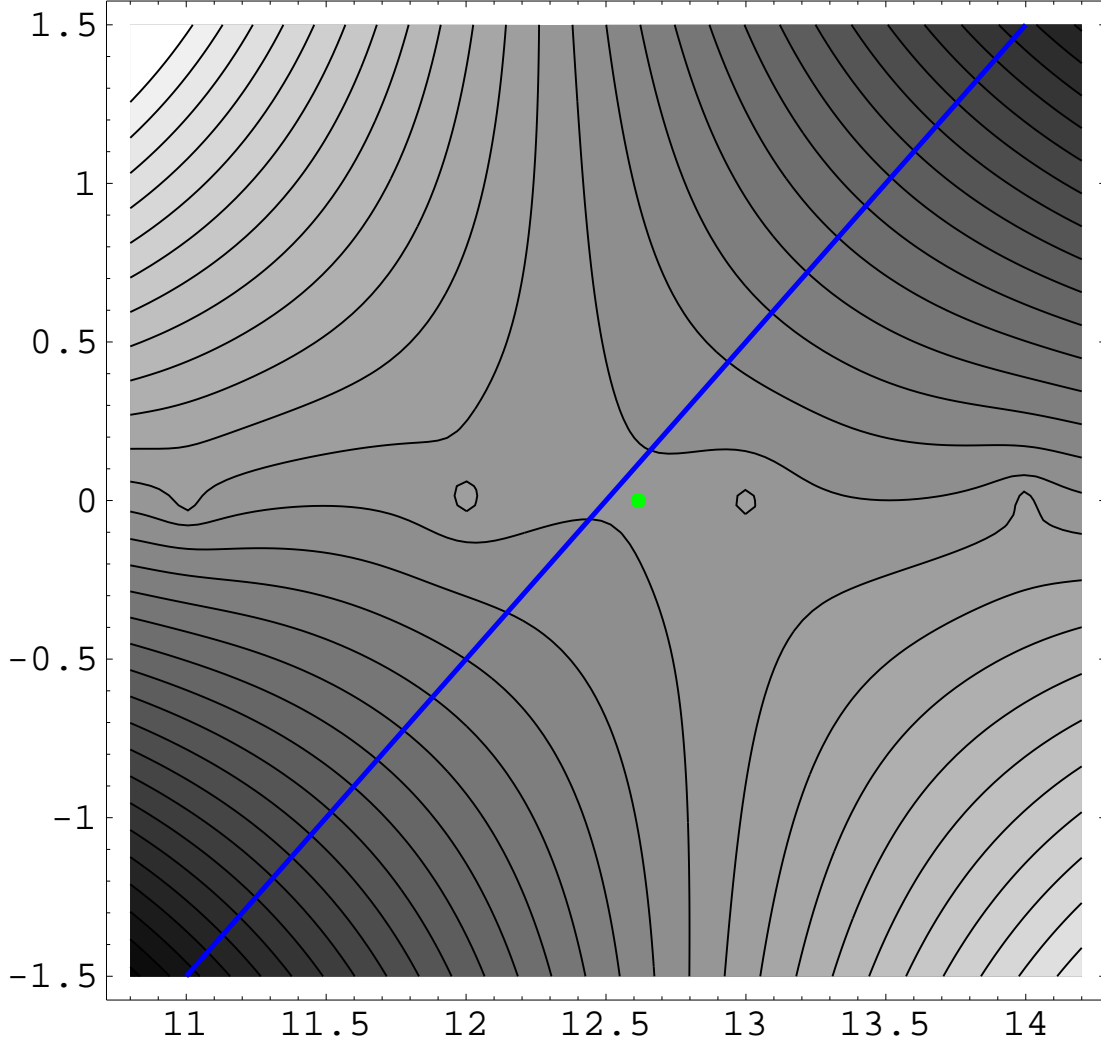
$$\log \left| \frac{\exp(i\pi z^2) z^{-s}}{e^{i\pi z} - e^{-i\pi z}} \right|$$



$$s = 1.5 + 1000i, N = 12$$

0 ↗ 1 and 12 ↗ 13

# Closeup View

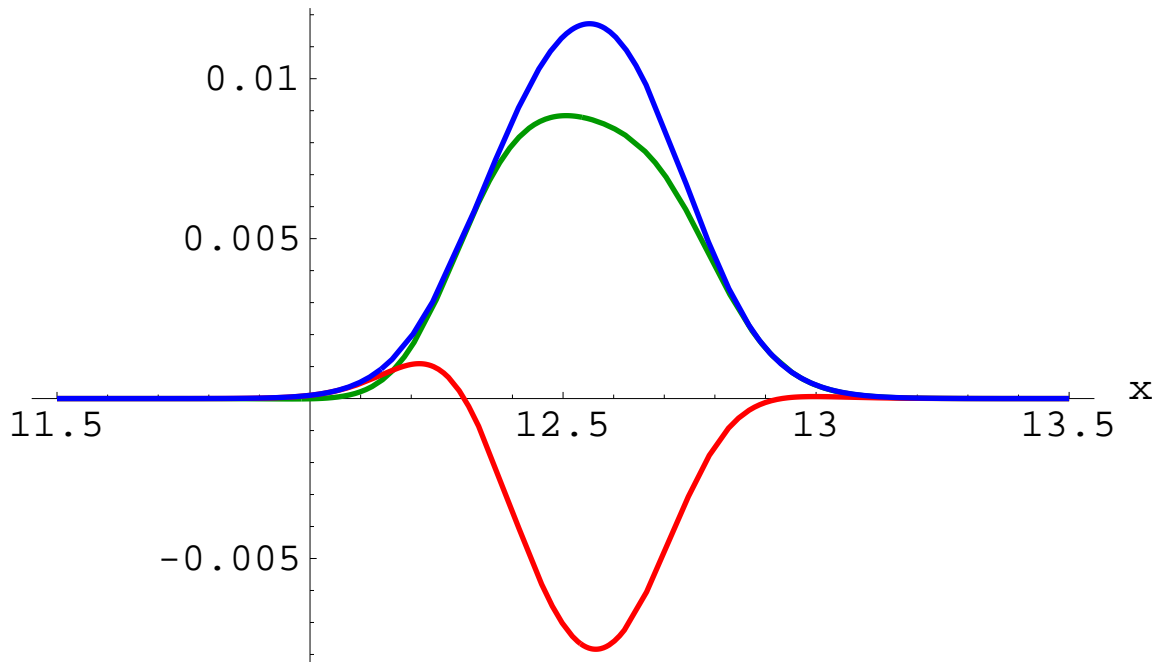


# The Integrand

Absolute Value, Real and Imaginary Parts of

$$f(s, z) = \frac{\exp(i\pi z^2) z^{-s}}{e^{i\pi z} - e^{-i\pi z}}$$

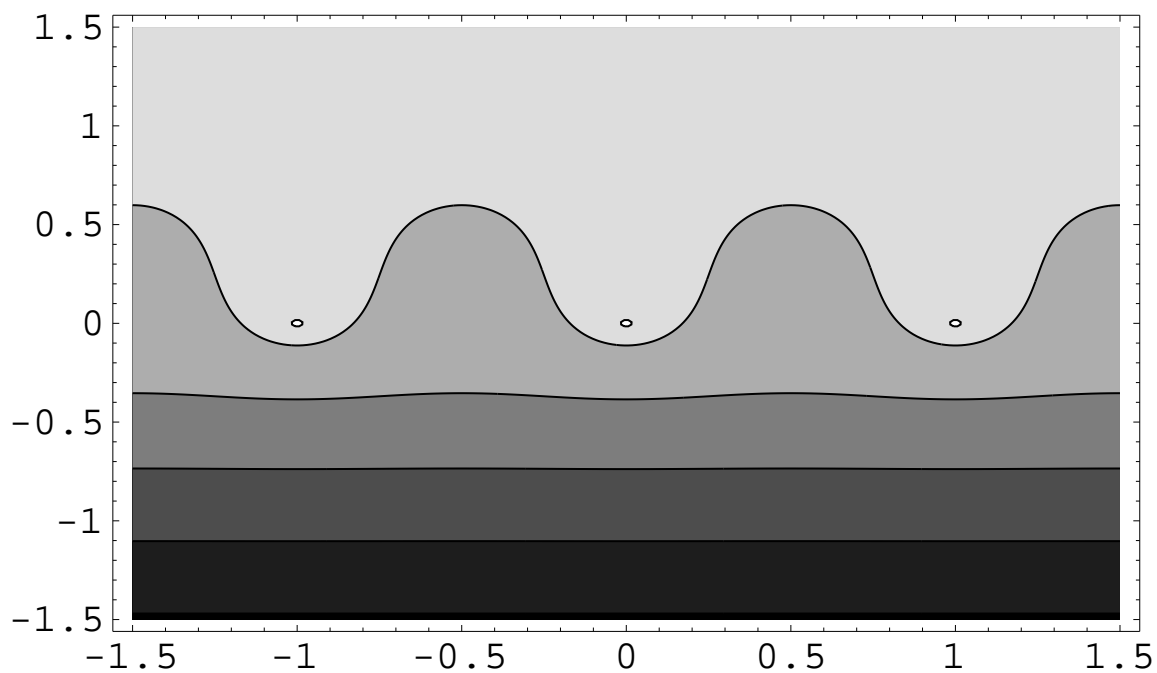
$$z = x + i(x - 12.5)$$



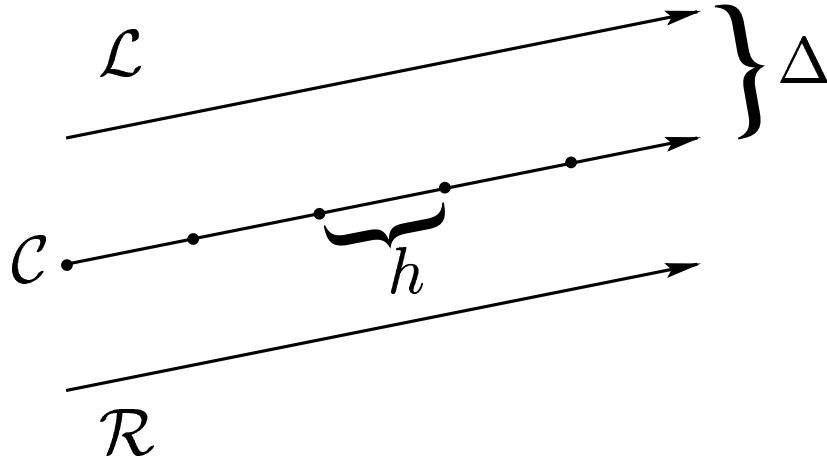
# Quadrature Analysis — a Tool

$$\text{Let } H(w) = \frac{1}{1 - e^{2i\pi w}}.$$

Note  $H(u - iv) = O(e^{-2\pi v})$  as  $v \rightarrow \infty$ .



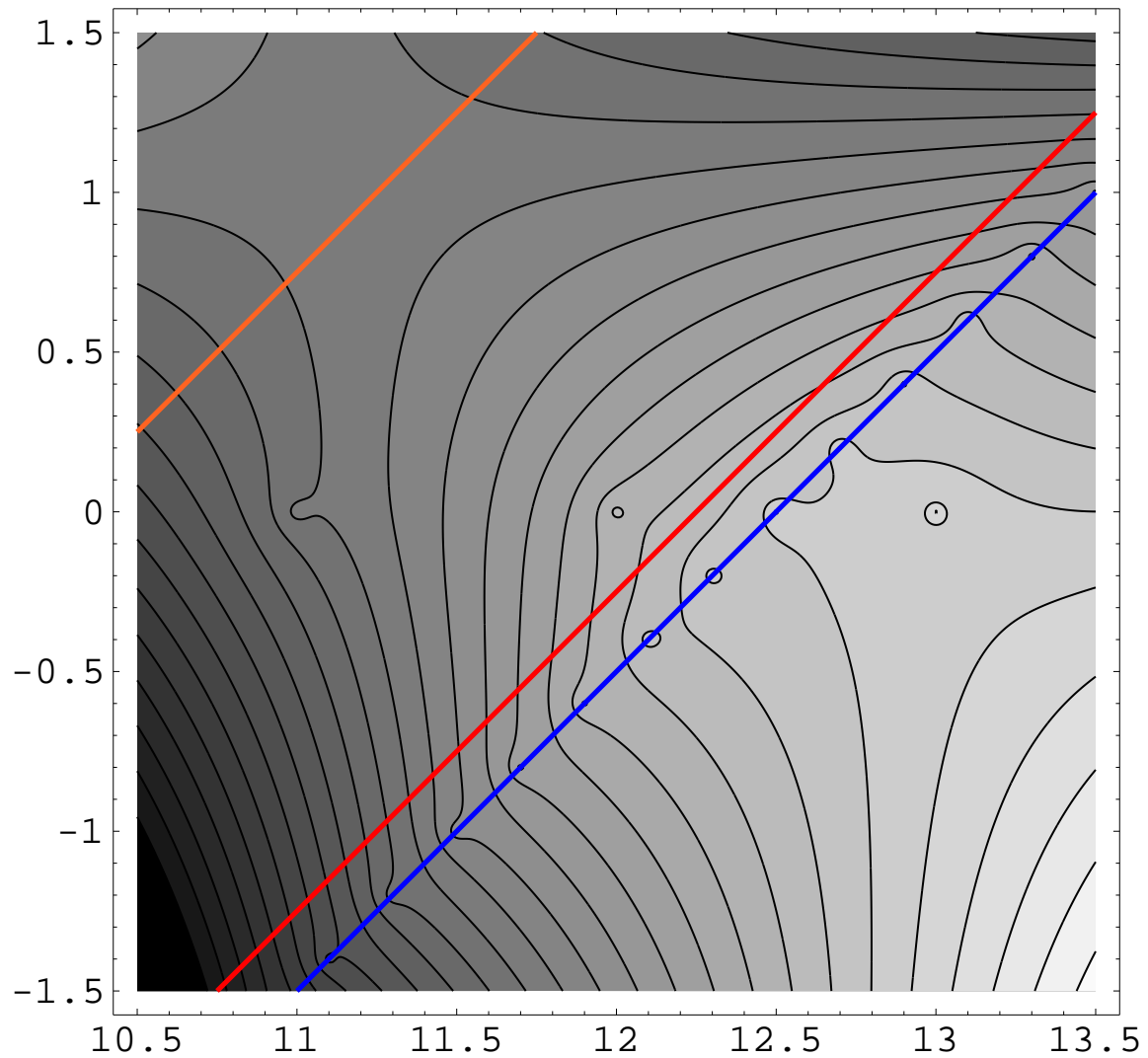
# A Quadrature Formula



$$\int_{\mathcal{C}} f(z) dz = h \sum_{m \in \mathbb{Z}} f(z_0 + m h) + \int_{\mathcal{L}} f(z) H((z_0 - z)/h) dz + \int_{\mathcal{R}} f(z) H((z - z_0)/h) dz,$$

Note  $\int_{\mathcal{L}} = O_{\Delta}(e^{-2\pi\Delta/|h|})$ , similarly for  $\int_{\mathcal{R}}$ .

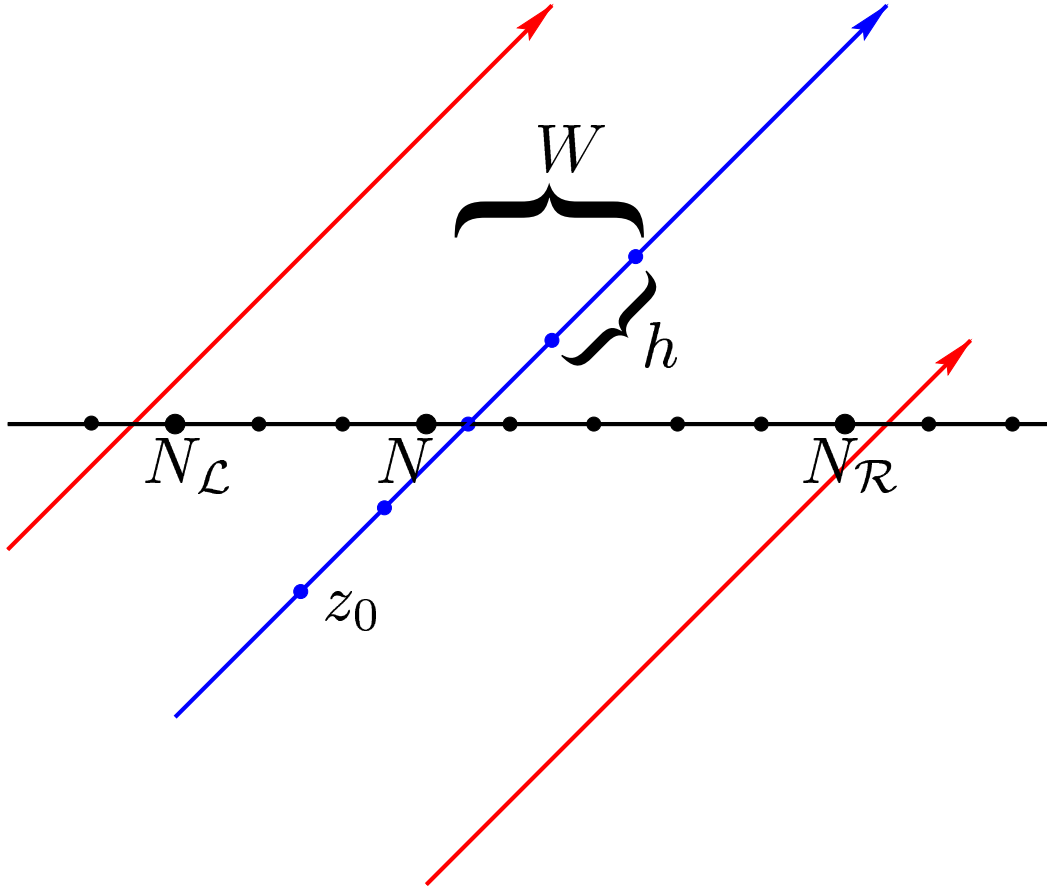
# “Left Error” for $I_0$ Integrand



$$h = 0.2(1 + i)$$

10 ↗ 10.5, 12 ↗ 12.5 and 12 ↗ 13

# 5 Parameters for Quadrature



$N_{\mathcal{L}}$ ,  $N$ ,  $N_{\mathcal{R}}$ ,  $W$ , and  $M$ , where  
 $2W =$  Width of sample interval, and with  
 $M + 1$  sample points

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$$z_0 = N + 1/2 - W(1 + i)$$

$$h = 2W(1 + i)/M$$

## Quadrature Formula for $I_0(s)$

$$\begin{aligned}
 I_0(s) &= \sum_{n=1}^N n^{-s} + h \sum_{m=0}^M f(s, z_0 + mh) \\
 &\quad - \sum_{n=N_{\mathcal{L}}}^N H((N + 1/2 - n)/h) n^{-s} \\
 &\quad + \sum_{n=N+1}^{N_{\mathcal{R}}} H((n - N - 1/2)/h) n^{-s} \\
 &\quad + O(e^{-2\pi W^2 + \epsilon}) + O(e^{-\pi KM/W})
 \end{aligned}$$

where

$$f(s, z) = \frac{\exp(i\pi z^2) z^{-s}}{e^{i\pi z} - e^{-i\pi z}} \quad \text{and}$$

$$K = \min(5/4 + N - N_{\mathcal{L}}, 1/4 + N_{\mathcal{R}} - N).$$



# Computing $\zeta(s)$ to 28 decimal places

$$s = 1/2 + 10^5 i$$

$$N = 126$$

$$N_{\mathcal{L}} = 121$$

$$N_{\mathcal{R}} = 131$$

$$W = 2.5$$

$$M = 50$$

Computation time using quadrature was 0.31 sec. in GP/PARI on a 300MHz Ultrasparc — vs 204 sec. (18 sec. after first computation) using PARI's built-in routine based on Euler-Maclaurin summation.

# Computing $\zeta(s)$ to 1000 decimal places

$$s = 1/2 + 10^5 i$$

$$N = 126$$

$$N_{\mathcal{L}} = 100$$

$$N_{\mathcal{R}} = 152$$

$$W = 13$$

$$M = 1500$$

Computation time using quadrature was 25 minutes in GP/PARI on 300MHz Ultrasparc.

# Things to do

- Get explicit, tight, error bounds.
- Do a more careful complexity analysis.
- Generalize to other zeta functions and  $L$ -functions.

# Literature

- For a good survey of methods for computing  $\zeta(s)$ , see the preprint [BBC].
- For a careful error analysis of the Euler-Maclaurin formula for  $\zeta(s)$ , see [CO92].
- For a careful error analysis of the Riemann-Siegel formula, when  $\sigma = 1/2$ , see [Gab79].
- Methods for efficient computation of  $\zeta(\sigma + it)$  at many equally spaced values of  $t$  are described in [OS88].
- For “smoothed” versions of the Riemann-Siegel formula, with better accuracy than the classical version, see [BK92].
- For further discussion of quadrature of saddle point integrals, see [Tem77].

# References

- [BBC] Jonathan M. Borwein, David M. Bradley, and Richard E. Crandall. Computational strategies for the Riemann zeta function. Preprint available at <http://www.cecm.sfu.ca/preprints/1998pp.html>.
- [BK92] Michael V. Berry and Jonathan P. Keating. A new asymptotic representation for  $\zeta(\frac{1}{2} + it)$  and quantum spectral determinants. *Proc. Roy. Soc. London Ser. A*, 437(1899):151–173, 1992.
- [CO92] Henri Cohen and Michel Olivier. Calcul des valeurs de la fonction zêta de Riemann en multiprécision. *C. R. Acad. Sci. Paris Sér. I Math.*, 314(6):427–430, 1992.
- [Gab79] Wolfgang Gabcke. *Neue Herleitung und Explizite Restabschätzung der Riemann-Siegel-Formel*. PhD thesis, Georg-August-Universität zu Göttingen, 1979.
- [Gal99] William F. Galway. *Implementing the Lagarias-Odlyzko Analytic Algorithm for  $\pi(x)$* . PhD thesis, University of Illinois at Urbana-Champaign, 1999. (expected).
- [LO87] J. C. Lagarias and A. M. Odlyzko. Computing  $\pi(x)$ : an analytic method. *Journal of Algorithms*, 8:173–191, 1987.

- [OS88] Andrew M. Odlyzko and A. Schönhage. Fast algorithms for multiple evaluations of the Riemann zeta function. *Trans. Amer. Math. Soc.*, 309:797–809, 1988.
- [Tem77] Nico M. Temme. *The numerical computation of special functions by use of quadrature rules for saddle point integrals. I. Trapezoidal integration rules*. Mathematisch Centrum, Amsterdam, 1977. Mathematisch Centrum, Afdeling Toegepaste Wiskunde, No. TW 164/77. [Mathematical Center, Department of Applied Mathematics, No. TW 164/77].